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Study of the proton chemical shifts and charge distribution in derivatives of aromatic carboxylic acids

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Abstract

1. The PMR spectra and conformations of dimethyl orthophthalate and dimethyl isophthalate were studied. 2. A theoretical estimation was made of the constants in the equation relating the value of the chemical shift to the charge distribution. 3. The experimental distribution of charge in dimethyl orthophthalate, dimethyl isophthalate, and methyl benzoate was obtained and is in qualitative agreement with the theoretical data. © 1970 Consultants Bureau.

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